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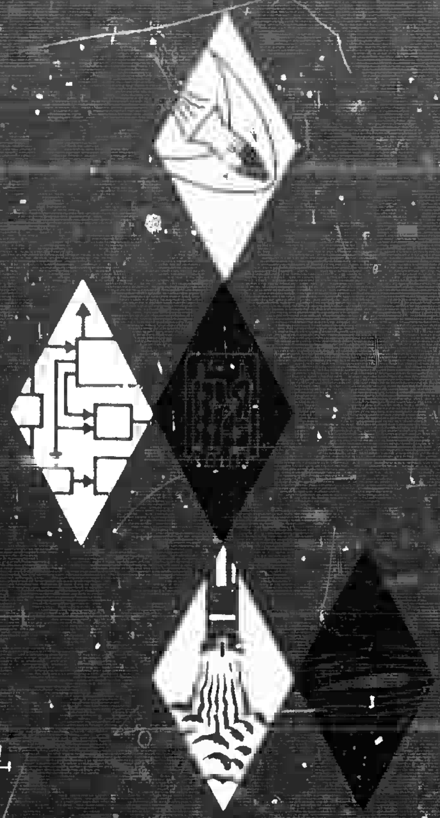

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TECHNICAL REPORT NO. 501

A FINITE-DIFFERENCE METHOD SOLUTION OF NON-SIMILAR, EQUILIBRIUM AND NON-EQUILIBRIUM AIR, BOUNDARY LAYER EQUATIONS WITH LAMIN AND TURBULENT VISCC ITY MODELS

PART I: ANALYSIS

(FINAL REPORT)

By H. E. Gould
L. S. Galowin

February 2, 1965

GENERAL APPLIED SCIENCE LABORATORIES, INC.
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ABSTRACT

An analysis is developed for the boundary layer flows, with dissociated and ionized air species in chemical equilibrium or with finite rate chemistry, about general body geometries at zero angle of attack. The partial differential equations for the boundary layer, about axisymmetric and two-dimensional bodies, are transformed to the von Mises stream function coordinate. The resulting equations are reduced to an algebraic system obtained by adopting an explicit finite-difference method of solution. These equations provide the basis for a computer program to obtain numerical solutions.

Laminar and several turbulent viscosity models are included in the analysis. Turbulent diffusivity models based upon the law of the wall, law of the wake, a curve-fit to pipe flow eddy viscosity and laminar viscosity contributions are introduced. Constant Prandtl, Lewis and Schmidt numbers through the thickness of the boundary layer are assumed. The thermodynamic and chemical kinetic data of the air species O_2, O, N_2, N, NO, NO^+, and e^- are considered. Provision is made in the program for solutions with either non-equilibrium, complete equilibrium, or finite rate chemistry with the wall in equilibrium.

Boundary layer swallowing of inviscid shock layer flow behind curved shocks is included. The streamwise variation in local outer edge conditions are obtained from an approximate inviscid streamline tracing procedure.

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LIST OF SYMBOLS

$A_1, A_2 \ldots$	control indicators for program problem selection
$B_1, B_2 \ldots$	turbulent viscosity coefficients
c_i	i^{th} species mass fraction
c_p	specific heat at constant pressure
$\mathcal{D}$	diffusional transport term of species equation
D_{ki}, D	diffusion coefficients
$\mathcal{E}^H, \mathcal{E}^C$	diffusional transport terms of energy equation
$H = h + \frac{u^2}{2}$	total enthalpy
h	static enthalpy
h_i	i^{th} species static enthalpy
k	thermal conductivity
$L = \frac{\rho D c_p}{k}$	mixture Lewis number
M_i	molecular weight of i^{th} species
m, n	reference column and row indicators of x, Ψ plane
p	static pressure
$P = \frac{c_p \mu}{k}$	Prandtl number
q_w	heat flux at the wall
r	body radius measured from centerline
R_o	universal gas constant

$R_{ex} = \frac{\rho_e u_e x}{\mu_e}$	Reynolds number based on edge conditions
$R_{ew} = \frac{\rho_w u_e x}{\mu_w}$	Reynolds number based on wall conditions
R_{CH}	channel height in two-dimensional flow
s	streamline coordinate from shock
$S = \frac{\rho D}{\mu}$	Schmidt number
T	temperature
u	velocity component in x-dire ion
v	velocity component in y-direction
$V_{i,y}$	diffusional velocity of i^{th} species in y-direction
$\dot{w}_i$	net rate of production of i^{th} species
x,y	curvilinear body coordinate system
Δx	x-wise grid division of x, Ψ plane
δ	boundary layer thickness
δ^*	displacement thickness
$\epsilon = 0,1$	selector for two-dimensional or axisymmetric selection
ζ_1 , ζ_2	reference cartesian coordinate system
θ	momentum thickness
$\varkappa$	empirical constants of turbulent eddy viscosities
μ	viscosity coefficient
ρ	density

$\bar{\sigma}$	differential equation coefficient of stability step-size requirement
τ	shear stress
Ψ	transformed (von Mises) normal coordinate
$\Delta\Psi$	Ψ-wise grid division of x,Ψ plane

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PART I: ANALYSIS

(FINAL REPORT)

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I. INTRODUCTION

An explicit finite-difference method solution has been studied for the equations of the boundary layer about hypersonic reentry vehicles in chemically reacting air. The coupling of the effects of finite-rate chemistry with various models for the diffusional phenomena in laminar and turbulent flows was reported previously, in Ref. 1. The computer program developed in the earlier effort was limited to the models of turbulent viscosity, and only permitted non-equilibrium calculations. A somewhat more generalized computational capability has been made available from the current investigation. This

report presents the results of this enlargement of effort.

The capability has been provided for solving the boundary layer equations with the multicomponent air system in equilibrium. The option of selecting the wall in equilibrium and the flow in non-equilibrium has been added; this eliminates the need to specify the wall species over the body as input. An enlarged selection of turbulent diffusivity models has also been included. Two terms of the series solutions for the analytic determination of wall parameters and derivatives of the functions in the vicinity of the wall have been adopted.

The pertinent boundary layer parameters for this work were defined in Ref. 1 and the methods of computation were also indicated there.

II. THE BOUNDARY LAYER EQUATIONS

The boundary layer equations for the steady flow of a chemically reacting, multicomponent gas mixture, neglecting radiative energy exchange and thermal diffusion, were transformed to the von Mises coordinates, x-Ψ. The transformation from the x-y plane is defined by

$$\rho u r^{\epsilon} = \frac{\partial \Psi}{\partial y} \quad ; \quad - \rho v r^{\epsilon} = \frac{\partial \Psi}{\partial x} , \tag{1}$$

where the body radius r(x) is measured normal to the centerline. This definition of the stream function, Ψ, automatically satisfies the continuity equation. The body radius appears for axisymmetric problems by setting $\epsilon = 1$ and for two-dimensional problems is eliminated with $\epsilon = 0$. The differential operators become, from (1),

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x} - \rho v r^{\epsilon} \frac{\partial}{\partial \Psi} \tag{1a}$$

and

$$\frac{\partial}{\partial y} = \rho u r^{\epsilon} \frac{\partial}{\partial \Psi} . \tag{1b}$$

The momentum equation in the transformed coordinates becomes

$$\frac{\partial u}{\partial x} = - \frac{1}{\rho u}\frac{\partial p}{\partial x} + r^{\epsilon}\frac{\partial \tau}{\partial \Psi} ; \qquad (2)$$

$$0 = \frac{\partial p}{\partial \Psi} , \qquad (2a)$$

where the shear stress is defined by

$$\tau = \rho u r^{\epsilon}(\mu^{L,T})\left(\frac{\partial u}{\partial \Psi}\right) . \qquad (3)$$

The viscosity coefficient, $\mu^{L,T}$, may be either the laminar or turbulent or the sum of both in the computer program developed from this analysis.

The total energy equation in the transformed plane becomes

$$\frac{\partial H}{\partial x} = r^{\epsilon}\frac{\partial}{\partial \Psi}(\mathcal{E}^{H} + \mathcal{E}^{C}) . \qquad (4)$$

The energy flux associated with the gradients of total enthalpy and kinetic energy is defined by

$$\mathcal{E}^{H} = \rho u r^{\epsilon}\left(\frac{\mu^{L,T}}{P^{L,T}}\right)\frac{\partial H}{\partial \Psi} + \rho u r^{\epsilon}(\mu^{L,T})\left(1 - \frac{1}{P^{L,T}}\right)\frac{\partial \frac{u^2}{2}}{\partial \Psi} . \qquad (5)$$

The Prandtl number, $P^{L,T}$, may be selected as any reasonable value for the gaseous mixture in either laminar or turbulent flows in the computer program. The energy flux associated with the diffusion velocity for each species is related by Fick's law to the gradient of the species mass fractions, c_i, and species enthalpy, and is expressed by

$$\mathcal{E}^C = \rho u r^{\epsilon} \left(1 - \frac{1}{L^{L,T}}\right) \left(\frac{1}{S^{L,T}}\right) (\mu^{L,T}) \sum_i h_i \frac{D_{ki}}{D} \frac{\partial c_i}{\partial \Psi} \qquad (6)$$

where D represents an effective average mixture (binary) diffusion coefficient. Laminar or turbulent Lewis numbers, $L^{L,T}$, and Schmidt numbers, $S^{L,T}$, may be specified in the computer program. The additional energy relationships required are the static enthalpy

$$h = H - u^2/2, \qquad (4a)$$

and the static enthalpy in terms of the species mass fractions and species enthalpies

$$h = \sum_i c_i h_i. \qquad (4b)$$

The species conservation equation in the transformed coordinates is

$$\frac{\partial c_i}{\partial x} = \frac{\dot{w}_i}{\rho u} + r^{\epsilon} \frac{\partial \mathcal{D}}{\partial \Psi}, \quad (i = 1,2,3,4...) \tag{7}$$

where the net rate of species production term, $\dot{w}_i$, is determined by the phenomenological law of mass action with the experimental reaction rates appropriate to the production of each chemical species. The term for the diffusion of species is given by

$$\mathcal{D} = \rho u r^{\epsilon} \left(\frac{\mu^{L,T}}{S^{L,T}}\right)\left(\frac{D_{k_i}^{L,T}}{D^{L,T}}\right)\frac{\partial c_i}{\partial \Psi} . \tag{8}$$

A dilute gas mixture has been assumed so that each species may be treated as an ideal gas; hence the partial pressure is

$$p_i = \rho_i \frac{R_o}{M_i} T , \tag{9a}$$

and the mixture density is given by

$$\rho = \frac{p}{RT \sum_i \frac{c_i}{M_i}} . \tag{9b}$$

III. CHEMISTRY, THERMODYNAMICS AND TRANSPORT PROPERTIES

The species considered in the (gas-phase) air reactions for the high temperatures of interest include O_2, O, N_2, N, NO, NO^+, and e^-. There are considered active in the following reactions (with catalyst C):

$$C + N_2 \rightleftarrows 2N + C \tag{10a}$$

$$C + O_2 \rightleftarrows 2O + C \tag{10b}$$

$$C + NO \rightleftarrows N + O + C \tag{10c}$$

$$NO + O \rightleftarrows N + O_2 \tag{10d}$$

$$N_2 + O \rightleftarrows NO + N \tag{10e}$$

$$N_2 + O_2 \rightleftarrows 2NO \tag{10f}$$

$$N + O \rightleftarrows NO^+ + e^- \tag{10g}$$

The reaction rates for the above reactions are the same as those of Ref. 1. (These laminar rates are also assumed to apply to the turbulent flows.)

Solution of the equations with finite-rate chemistry requires the evaluation of the net rate of production of species, $\dot{w}_i$, from the law of mass action with experimental reaction rates for production of each chemical species. The equations are the same as those of Ref. 1. In order to analyze equilibrium chemical systems, the equilibrium mass action laws, rather than the

conservation equations (7), must be solved for the species mass fractions. The equilibrium system of equations for the seven air species considered are taken from Ref. 2.

The conservation equations contain the transport properties of viscosity, thermal conductivity, and diffusivity as functions of the flow variables (e.g. temperature, pressure, and species mass fractions). The introduction of the nondimensional (constant) transport parameters of Prandtl, Lewis, and Schmidt numbers requires that only the viscosity must be formulated explicitly. The temperature dependency expressed by the Sutherland relationship will be utilized for the air in laminar flow. Theoretical descriptions of the turbulent flow structure are still inadequate. The analytical basis for turbulent boundary layer viscosity models is dependent upon semi-empirical correlations. Although details differ, there is a general acceptance of the characterization of turbulent layers divided into two regions, viz., an inner region close to the wall, and an outer region away from the wall, with different eddy viscosity models. The viscosity model over the inner region of the flow is usually taken as a law of the wall, and over the outer region as a law of the wake. Several turbulent viscosity models are provided within the computer

program (discussed in Part II) to permit combinations to be selectively controlled. Division of the turbulent boundary layer flow into a near wall region with one viscosity model, and an outer region with another viscosity model, will be controlled by a thickness ratio factor.

IV. METHOD OF SOLUTION - FINITE DIFFERENCE EQUATIONS

Solution of the system of equations discussed in Section II by an explicit finite-difference method was adopted for computer programming. The finite-difference formulation was established by employing the explicit difference relations, for the characteristic function F, as follows:

$$\frac{\partial F}{\partial x} = \frac{F(x+\Delta x, \Psi) - F(x, \Psi)}{\Delta x} \; ; \tag{11a}$$

$$\frac{\partial F}{\partial \psi} = \frac{F(x, \Psi + \Delta \Psi) - F(x, \Psi - \Delta \Psi)}{2\Delta\Psi} \; ; \tag{11b}$$

and

$$\frac{\partial}{\partial \Psi}\left[a \frac{\partial F}{\partial \Psi}\right] = \frac{a\left(x, \Psi + \frac{1}{2}\Delta\Psi\right)\{F(x, \Psi + \Delta\Psi) - F(x, \Psi)\}}{(\Delta\Psi)^2} - \frac{a\left(x, \Psi - \frac{1}{2}\Delta\Psi\right)\{F(x, \Psi) - F(x, \Psi - \Delta\Psi)\}}{(\Delta\Psi)^2} \, , \tag{11c}$$

where

$$a\left(x, \Psi \pm \frac{1}{2}\Delta\Psi\right) = \frac{1}{2}\left[a(x, \Psi \pm \Delta\Psi)\right] \, . \tag{11d}$$

The system of algebraic expressions derived from these differential equations is subjected to stability conditions requiring restrictions on the permissible grid dimensions.

The stability requirements cannot be precisely formulated for the nonlinear system of equations. However, on the basis of linear theory (see, e.g., Ref. 3) and subsequent numerical testing, the stability conditions applicable to the problem can be established. The analytical stability requirement from linear theory is

$$\frac{\bar{\sigma}\,\Delta x}{(\Delta\Psi)^2} \le \frac{1}{2}\,, \tag{12}$$

where $\bar{\sigma}$ indicates the average value of the locally quasi-constant coefficients from the linearized equations. The expressions for $\bar{\sigma}$ from the conservation equations are:

<u>Momentum</u>

$$\bar{\sigma}_u = r^{2\epsilon}\rho u(\mu^{L,T}) \;; \tag{12a}$$

<u>Energy</u>

$$\bar{\sigma}_H = r^{2\epsilon}\rho u\left(\frac{\mu^{L,T}}{P^{L,T}}\right) ; \tag{12b}$$

<u>Species</u>

$$\bar{\sigma}_{c_i} = r^{2\epsilon}\rho u\left(\frac{\mu^{L,T}}{S^{L,T}}\right)\left(\frac{D_{k_i}}{D}\right) . \tag{12c}$$

V. BOUNDARY CONDITIONS

The solution of the boundary layer equations requires that the initial distributions of velocity, total enthalpy and species mass fractions be specified; also, the boundary conditions at the wall and outer edges are required. At the wall the boundary conditions may be stipulated in terms of the normal gradients of the functions, rather than the functional values; in the case of the wall boundary condition of species, the element mass fractions must be conserved. (This arises from considerations of species diffusional velocities at the wall.) Values at the inviscid outer edge of the layer are not known a priori, but are derived from the boundary-layer swallowing of inviscid flow streamlines (computed within the program) as the calculation progresses in the streamwise direction. A streamline tracing procedure for swallowing behind curved shocks, based upon a linear variation of pressure with distance from the shock to the body station, will be used to determine the inviscid flow properties.

For convenience, a fixed reference coordinate system will be adopted to provide the geometrical descriptions of the body contours, shock geometry, relationship of the body with respect to the shock, and determination of shock-streamline intersection

points. Various combinations of spherical sections, ogives, cones, cylinders, flat plates, and wedge contours will provide the description of many body shapes. The shock shape will be based upon combinations of parabolas and straight-line segments for curve fits.

The pressure distribution about the body is required; the source of such data may be experimental, or analytically determined values from solution of the inviscid flow field may be used. Several equations will be provided to curve-fit the pressure distribution over the various geometrical regions.

VI. SERIES SOLUTION NEAR THE WALL

The introduction of the transformation variable, Ψ, results in a system of equations which contain a singularity at the wall as a result of the vanishing velocity, $u \to 0$. In Ref. 1 the method was discussed, for treating the singularity by developing series solutions in powers of $\Psi^{n/2}$ (which satisfy the differential equations) for the variables u, H, and c_i; the coefficients of the series were also shown as explicit functions of the flow properties. Utilization of the series solutions provides for the analytical evaluation of the slopes at the wall; these slopes are required in order to obtain the shear and heat transfer at the wall.

The finite-difference method adopted for solution of the system of equations requires accurate representation for the gradients of the dependent variables. A straightforward point-wise differencing method in the Ψ direction between the wall and first mesh point does not provide sufficient accuracy for the calculations. The slopes in this region are formulated analytically from the series solution. The coefficients of the series are determined by fitting to the computed values of the variables determined from the solution along the mesh lines of constant Ψ. Terms to the first power of Ψ will be retained so that only two coefficients of the series need to be evaluated after each (incremental) streamwise step.

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